

Order-Parameter Anisotropies in the Pnictides - An Optimization Principle for Multi-Band Superconductivity

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Using general arguments of an optimization taking place between the pair wave function and the repulsive part of the electron-electron interaction, we analyze the superconducting gap in materials with multiple Fermi-surface (FS) pockets, with exemplary application to two proto-type ferropnictide setups. On the basis of functional renormalization group (FRG) calculations for a wide parameter span of the bare interactions, we show that the symmetry of the gap and the nodal versus nodeless behavior is driven by this optimization requirement.

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The discovery of superconductivity (SC) in new compounds such as the iron pnictides has opened up a new avenue for studying the fundamental question "what is universal and what is material-dependent" concerning the mechanism of high- T_c SC in a wider class of materials other than, but also including, the cuprates. There, after more than two decades of intense research, more and more theoretical as well as experimental studies support a scenario where the general nature of the d -wave SC as well as other salient features are accounted for by an electronic pairing mechanism extracted from a one-orbital Hubbard model [1, 2] with the addition that the material-dependence is embedded in the multi-orbital (e.g. 3-band) extensions [3].

In other SC compounds such as the pnictides, however, the picture seems more complicated: Here, at the outset, multi-band SC appears with gaps possibly displaying different symmetries such as extended (sign-reversing) s -competing with d -wave and with nodal or also nodeless behavior on the disconnected Fermi surface (FS) sheets [4–16, 21, 22]. Accordingly, even the simplest multi-band Hamiltonian with only on-site interactions contains four possibly relevant terms, the intra-orbital and inter-orbital repulsion as well as the Hund's-rule coupling and pair hopping. Searching for SC pairing, these interactions have to be augmented with the orbital dependence of the FS pockets, since the interactions become matrices formed by local orbitals which have a dominant orbital "weight" at the FS pockets. We hence investigate whether this intricate interplay of multi-orbital band structure, FS topology and interactions still allows for insights into a more universal than material-dependent understanding of SC in these systems.

In this Letter, we describe an "optimization principle" which can help providing such a more universal picture. The main point of our work is to show that the SC state, its gap, and, in particular, its anisotropy in momentum space is determined by an optimization *which determines and optimizes the interplay between the at-*

tractive interaction in the SC-channel and the Coulomb repulsion. This optimization problem, as discussed below, is unavoidable in a multi-band SC situation: for the pnictides, it appears because of a frustration in the s_{\pm} -channel, when more than two FS-pockets are involved in setting up the pairing interaction.

Already from the BCS gap equation, one can see that Coulomb repulsion at a finite momentum transfer can induce pairing only when the wave vector of such an interaction connects regions on one FS (in the cuprate case), or regions on different FSs (in the pnictide case), which have opposite signs of the SC order parameter. This corresponds to putting the electron pairs in an anisotropic wave function such as d -wave in the high- T_c cuprates, or the sign-reversing s -wave (s_{\pm}) in the pnictides, where in the latter case the wave vector $(\pi, 0)$ in the unfolded Brillouin Zone connects hole (h) and electron (e) FS-pockets with a sign-changing s_{\pm} gap [4, 8]. Early studies based on either RPA spin-fluctuations (SF) scenarios [4] or on Renormalization-Group [RG] studies [8] of just one-hole and one-electron FS have reported a momentum-independent s_{\pm} gap. At first glance, this similarity of the gap function obtained by so dissimilar approaches as RPA and FRG may appear surprising. Indeed, the repulsive part of the Coulomb interaction is treated differently which leads to differing results for the general multi-pocket case [17].

The interesting setup for the optimization principle concerns a multi-pocket situation - as generally appearing in the ferro pnictides - where more than two pockets create crucial pairing interactions. In order to illustrate the principle at work for such a scenario, we investigate a 4-pocket and a 5-pocket Fermi surface (pFS) topology originating from a 5-band model (Fig. 1), and discuss the superconducting order parameter from that perspective.

The principal physical content of this optimization scenario can already be observed for the 4pFS and 5pFS scenarios in Figs. 1a and b. Let us try to understand the systems from the unfrustrated s_{\pm} limit where the

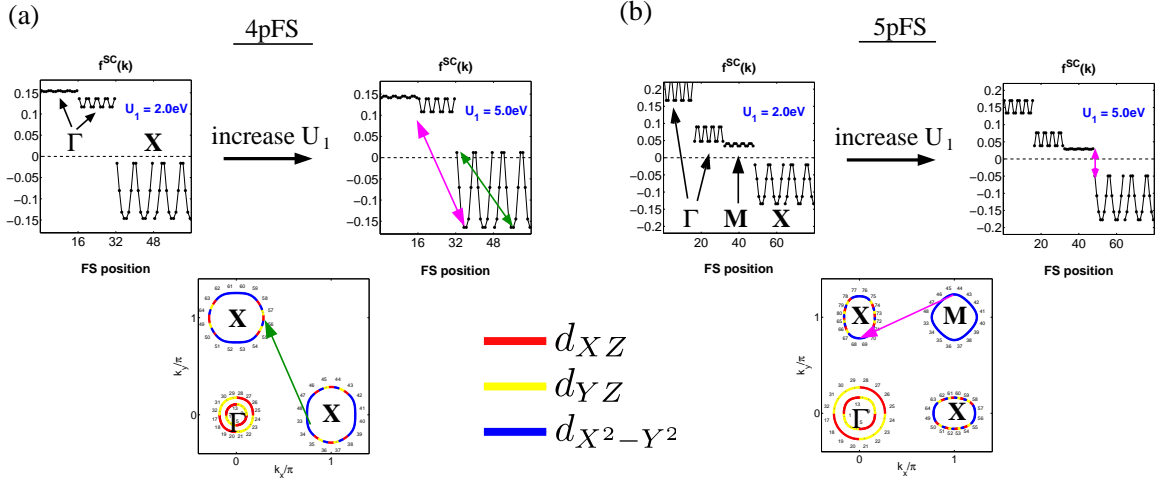


FIG. 1. (Color online). Scan of the intra-orbital interaction U_1 for both the 4pFS (Fig. 1a) and 5pFS (Fig. 1b) situations. Colors on the FS-pockets give dominant orbital weights, with dashed segments signalling several leading contributions. The increase of U_1 leads to an increase of the e-pocket gap for the 5pFS scenario, while it favors the nodal scenario for 4pFS.

$\Gamma \leftrightarrow X$ pair scattering between h-pockets at $\Gamma(0,0)$ and 3-pockets at $X(\pi,0)$ is minimized. Here, a green arrow for $X \leftrightarrow X$ scattering (4pFS, lower FS display in Fig. 1a) and a magenta arrow (5pFS) for $X \leftrightarrow M$ indicate additional interactions (dependent on the dominant orbital weights on the FSs). The green interaction in Fig. 1a frustrates the previous pure s_{\pm} limit. The system then strikes a compromise - and this is the essence of the optimization principle - by enhancing the anisotropy of the gap function (denoted by $f^{\text{SC}}(\mathbf{k})$ in Fig. 1) on the e-pockets at X (FS positions 32 to 64 in Fig. 1), eventually reaching even a nodal situation for larger interactions. The dominant part of the $X \leftrightarrow X$ interaction acts so as to push the peaks of the e-gap function further up, while the dominant part of the ($\Gamma \leftrightarrow X$) interaction (magenta arrow in Fig. 1a) tries to push the e-gap valleys down. Thus, a transparent understanding of the anisotropies and the nodeless versus nodal behavior emerges: the multi-band SC adjusts the momentum dependence of the gap, i.e. its anisotropy, so as to minimize the effect of the Coulomb repulsion [18].

In more mathematical terms, this optimization is reflected in Eq. 5 below for the dominant Cooper-channel eigenvalue $c_1^{\text{SC}}(\Lambda)$ taking the largest negative value:

$$c_1^{\text{SC}}(\Lambda) = \langle f^{\text{SC}}(\mathbf{k}) V_{\Lambda}^{\text{SC}}(\mathbf{k}, -\mathbf{k}, \mathbf{p}) f^{\text{SC}}(\mathbf{p})^* \rangle \quad (1)$$

Here, as detailed in Eq. 5, V_{Λ}^{SC} denotes the pairing function, where Λ is the RG-flow parameter and $f^{\text{SC}}(\mathbf{k})$ the SC (gap) form factor associated with it. $\langle \dots \rangle$ denotes the inner product and involves the \mathbf{k} - and \mathbf{p} -points on all 4 (or 5) FS-pockets (Fig. 1). We have

$$c_1^{\text{SC}}(\Lambda) = \sum_{\text{FS } l,m} c_{l,m}^{\text{SC}}(\Lambda), \quad (2)$$

and its largest negative value is determined via an optimization taking place between all pockets l and m . This

is a frustration problem as not all minimization conditions can be fulfilled at the same time.

In conjunction with the underlying FS topology obtained from LDA-type calculations [5], our FRG-studies also serve to answer which of the four intrasite interactions in the starting Hamiltonian are playing a leading role. To this extent, we report on an extensive parameter-sweep study the results of which are fully in line with the optimization argument. Placing the value of these interactions finally around the spread of values obtained in recent ab-initio DFT work [20], we find the intra-orbital interaction U_1 to take on the pivotal role. The 4pFS and 5pFS scenarios can be cast into a 5-band model, with

$$H_0 = \sum_{\mathbf{k},s} \sum_{a,b=1}^5 c_{\mathbf{k}as}^{\dagger} K_{ab}(\mathbf{k}) c_{\mathbf{k}bs}. \quad (3)$$

Here c 's stand for electron annihilation operators, a, b for the d -orbitals, and s denote the spin indices.

In the many-body part the intra- and inter-orbital interactions U_1 and U_2 , as well as the Hund's coupling J_H and the pair hopping J_{pair} enter, i.e.

$$H_{\text{int}} = \sum_i \left[U_1 \sum_a n_{i,a\uparrow} n_{i,a\downarrow} + U_2 \sum_{a<b,s,s'} n_{i,as} n_{i,bs'} + \sum_{a<b} (J_H \sum_{s,s'} c_{ias}^{\dagger} c_{ibs'}^{\dagger} c_{ias'} c_{ibs} + J_{\text{pair}} c_{ia\uparrow}^{\dagger} c_{ia\downarrow}^{\dagger} c_{ib\downarrow} c_{ib\uparrow}) \right], \quad (4)$$

where $n_{i,as}$ denote density operators at site i of spin s in orbital a . Typical interaction settings are dominated by intra-orbital coupling, $U_1 > U_2 > J_H \sim J_{\text{pair}}$, and can be obtained from constrained RPA calculations [20].

Details of the electronic structure such as the FS topology and, more specifically, the presence of the (π, π) -pocket are crucial for the SC state [4–16]. Using FRG on

the above 5-band (Fe d -orbital) model of the Fe-based SC with orbital interactions as in Eq. 3 and 4, we have recently found that the gap on the e-pockets can undergo a nodal transition if the h-pocket at (π, π) is absent [15]. Similar conclusions have been reached by Maiti and Chubukov using a parquet RG analysis [21]. On the basis of RPA calculations, Kuroki et al. [5] using a similar Hamiltonian as in Eqs. 3 and 4 have already argued that the (π, π) -pocket is sensitive to the lattice structure ("pnictogen height") and crucial for the gap structure. Kemper et al. [16], within again a 5-orbital RPA theory, further substantiated these conclusions. In particular, they demonstrated the sensitive dependence of the SC state to aspects of the electronic structure such as the FS topology and the FS orbital weights.

In the FRG [9–11, 15, 23], one starts from the bare many-body interaction (Eq. (2)) in the Hamiltonian and the pairing is dynamically generated by systematically integrating out the high-energy degrees of freedom including important fluctuations (magnetic, SC, screening, vertex corrections) on equal footing. This differs from the RPA which takes right from the outset a magnetically driven SF-type of pairing interaction.

For a given instability characterized by some order parameter $\hat{O}_{\mathbf{k}}$, the 4-point function (4PF) $V_{\Lambda}(\mathbf{k}_1, \mathbf{k}_2, \mathbf{k}_3, \mathbf{k}_4)$ in the particular ordering channel can be written in shorthand notation as $\sum_{\mathbf{k}, \mathbf{p}} V_{\Lambda}(\mathbf{k}, \mathbf{p}) [\hat{O}_{\mathbf{k}}^{\dagger} \hat{O}_{\mathbf{p}}]$ [12]. Accordingly, the 4PF $V_{\Lambda}(\mathbf{k}, -\mathbf{k}, \mathbf{p}, -\mathbf{p})$ in the Cooper channel can be decomposed into different eigenmode contributions [9, 15]

$$V_{\Lambda}^{\text{SC}}(\mathbf{k}, \mathbf{p}) = \sum_i c_i^{\text{SC}}(\Lambda) f^{\text{SC}, i}(\mathbf{k})^* f^{\text{SC}, i}(\mathbf{p}), \quad (5)$$

where i is a symmetry decomposition index, and the leading instability of that channel corresponds to an eigenvalue $c_1^{\text{SC}}(\Lambda)$ first diverging under the flow of Λ . $f^{\text{SC}, i}(\mathbf{k})$ is the SC form factor of pairing mode i which tells us about the SC pairing symmetry and hence gap structure associated with it. In FRG, from the final Cooper channel 4PFs, this quantity is computed along the discretized Fermi surfaces (as shown in Fig. 1), and the leading SC instabilities are plotted in Figs. 1 to 3. If not stated differently, the interaction parameters not specified in the plots are kept fixed at the representative setup $U_1 = 3.5\text{eV}$, $U_2 = 2.0\text{eV}$, $J_{\text{H}} = J_{\text{pair}} = 0.7\text{eV}$.

We first investigate the behavior upon the variation of the intraorbital interaction scale U_1 (Fig. 1). For small values of U_1 ($U_1 = U_2 = 2\text{eV}$) in Fig. 1a, the s_{\pm} -sign change is induced by the "optimization principle" between the h-pockets around the Γ -point and the e-pockets around the X points. By increasing U_1 , the 4pFS system develops a pronounced gap anisotropy at the electron pockets, which eventually leads to gap nodes at $U_1 \sim 3\text{eV}$ (Fig. 1a). This behavior is due to an enhanced U_1 repulsion within the $d_{X^2-Y^2}$ orbitals, which amplifies the pair scattering within the $d_{X^2-Y^2}$ -dominated parts of one electron pocket to the other (see green arrow in Fig. 1a

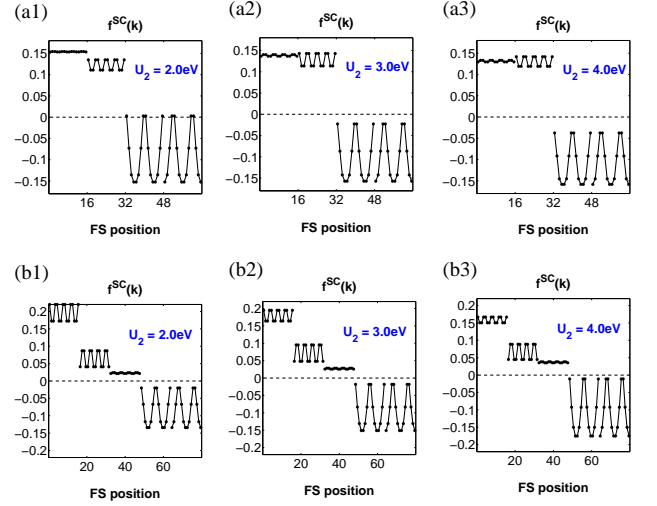


FIG. 2. (Color online). Scan of U_2 . Upon increase, more and more relevant scattering contributions from the 3rd hole pocket (M) in the 5pFS scenario (row (b)), to parts of the electron pockets of different orbital content increase the anisotropy. In the 4pFS scenario (row (a)), the anisotropy decreases due to a weakening of the previously dominant scattering between the peaks and valleys of the e-pockets.

for $U_1 = 5\text{eV}$). The above mentioned optimization requirement between a repulsive interaction and the pair wave function then favors an increased gap anisotropy between the peak and the valley of the SC gap on the e-pockets, which eventually yields a sign change.

In the 5pFS scenario (Fig. 1b), the additional M -pocket, which exclusively carries $d_{X^2-Y^2}$ orbital weights, also generates pair scatterings due to U_1 to the $d_{X^2-Y^2}$ -dominated parts of the electron pockets (see magenta arrows in Fig. 1b). This pushes down the peaks (tips) of the SC-gap on the electron pockets, on the basis of the same orthogonality argument (magenta arrow in Fig. 1b).

As the inter-orbital interaction U_2 is increased (Fig. 2), the main change is that the significance of the $d_{X^2-Y^2}$ scatterings driven by U_1 is slightly lowered. As the interorbital scattering phase space becomes important, the orbital distribution along the pockets determines more and more the behavior. For the 5pFS scenario (row (b) in Fig. 2), this gives an increased e-pocket anisotropy and a smaller e-pocket gap. For the 4pFS scenario, the nodal propensity is significantly reduced, as the previously decisive scattering between the peaks and the valleys of the electron pockets becomes less relevant.

As J_{H} is increased, similar to Wang et al. [13], we observe that the anisotropy on the e-pockets is enhanced, again because of the general orthogonality requirement between the repulsive interaction and the SC pair state, which applies both to 5pFS and 4pFS scenarios. Within a reasonable parameter range up to $\sim 1\text{eV}$, the modification of the SC form factor is comparably small.

On the bare level, J_{pair} gives a positive semidefinite

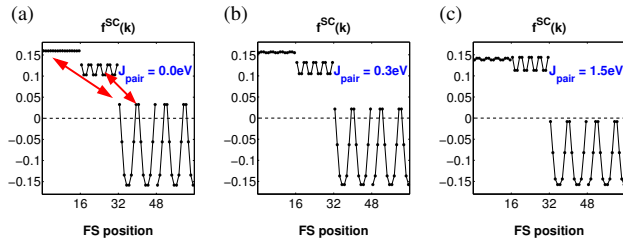


FIG. 3. (Color online). Scan of J_{pair} . The increase of pair-hopping helps to drive a gap for the 4pFS.

contribution to the Cooper channel. As a consequence, it increases the absolute Cooper channel scale and leads to an increase of the Λ -divergence scale of the SC instability (not shown here). While the SC form factor for the 5pFS scenario remains essentially unchanged, we observe some decrease of nodal propensity in the 4pFS scenario (see Fig. 3). There, the J_{pair} scattering contribution between the Γ hole pockets and the tips of the electron pockets play a similar role as the scattering contribution of the 5th hole pockets in the 5pFS scenario. However, this scattering takes place now between $d_{XZ} \rightarrow d_{X^2-Y^2}$ and $d_{YZ} \rightarrow d_{X^2-Y^2}$, orbitals (red arrows in Fig. 3).

In summary, we have demonstrated the usefulness of the optimization principle to provide a more universal characterization of gap anisotropies in multi-band SC. The optimization minimizes the Coulomb repulsion, which is needed because of frustration (such as occurring in the s_{\pm} -channel in our example), when more than two FS-sheets are contributing to the pairing interaction. Using FRG for two generic FS topology setups of the pnictides, we show that the optimization principle relates the gap anisotropies and their nodeless versus nodal behavior in a rather transparent way to the multi-orbital band structure, FS topology, and interactions.

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